

Supporting Information

“The CN_7^- Anion”

Thomas M. Klapötke^{,[a]} and Jörg Stierstorfer^[a]*

^{*,a} Department Chemistry and Biochemistry, Energetic Materials Research, Ludwig-Maximilian University of Munich, Butenandtstr. 5-13, D-81377 Munich, Germany, phone:

+49 89 2180 77491; fax: + 49 89 2180 77492; tmk@cup.uni-muenchen.de

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X-ray tables

Table S1. Bond distances (Å) of the CN_7^- anions of compounds **2** - **6**

atoms	1	2	3	4a	4b	5a	5b	6
N1–N2	1.372(2)	1.348(2)	1.358(4)	1.354(3)	1.356(3)	1.351(4)	1.353(4)	1.349(2)
N2–N3	1.295(2)	1.317(2)	1.306(4)	1.300(3)	1.308(3)	1.309(4)	1.306(4)	1.315(2)
N3–N4	1.355(2)	1.352(2)	1.360(4)	1.347(3)	1.348(3)	1.359(4)	1.364(4)	1.347(2)
C1–N1	1.321(2)	1.330(2)	1.316(4)	1.319(3)	1.330(3)	1.319(4)	1.335(4)	1.335(2)
C1–N4	1.327(2)	1.327(2)	1.337(5)	1.329(3)	1.310(3)	1.333(4)	1.314(4)	1.338(2)
C1–N5	1.383(2)	1.409(2)	1.401(5)	1.403(3)	1.412(3)	1.406(5)	1.393(4)	1.390(2)
N5–N6	1.267(2)	1.252(2)	1.250(4)	1.246(3)	1.251(3)	1.255(4)	1.259(4)	1.259(2)
N6–N7	1.117(2)	1.123(2)	1.125(4)	1.103(3)	1.120(3)	1.128(4)	1.125(4)	1.121(2)

Table S2 Bond distances (Å) of the CN_7^- anions of compounds **7** - **10**

atoms	7a	7b	8	9	10a	10b	10c
N1–N2	1.354(3)	1.354(3)	1.354(3)	1.354(6)	1.360(4)	1.348(4)	1.359(4)
N2–N3	1.317(3)	1.313(3)	1.316(3)	1.316(5)	1.309(4)	1.327(4)	1.306(4)
N3–N4	1.349(3)	1.350(3)	1.352(3)	1.355(6)	1.354(4)	1.351(4)	1.356(4)
C1–N1	1.317(4)	1.330(4)	1.324(3)	1.336(6)	1.330(4)	1.330(4)	1.326(4)
C1–N4	1.327(4)	1.323(4)	1.328(3)	1.315(5)	1.331(4)	1.330(4)	1.329(4)
C1–N5	1.407(4)	1.410(4)	1.411(3)	1.411(6)	1.411(4)	1.400(4)	1.405(4)
N5–N6	1.255(3)	1.255(3)	1.264(3)	1.244(6)	1.265(4)	1.257(4)	1.257(5)
N6–N7	1.117(4)	1.120(4)	1.112(3)	1.138(5)	1.119(4)	1.111(5)	1.127(5)

Table S3 Selected bond angles (°) of the CN_7^- anions of compounds **2** - **6**

atoms	1	2	3	4 a	4b	5a	5b	6
N1–C1–N4	109.5(2)	114.0(1)	114.3(4)	113.7(2)	113.9(2)	113.7(3)	114.8(3)	112.6(2)
N1–C1–N5	121.0(1)	121.1(1)	126.8(4)	127.3(2)	126.6(2)	125.9(4)	125.6(3)	127.47(14)
N4–C1–N5	129.5 (2)	125.0(1)	118.9(3)	119.0(2)	119.4(2)	120.4(3)	119.6(3)	119.91(14)
C1–N5–N6	113.1(1)	113.7(1)	114.2(3)	115.2(2)	112.6(2)	112.9(3)	116.1(3)	114.6(1)
N5–N6–N7	171.9(2)	172.3(2)	171.5(3)	169.8(3)	175.0(3)	172.5(4)	172.3(4)	170.7(2)
N1–C1–N5–N6	174.7(1)	176.5(1)	-0.7(7)	-5.7(4)	-176.5(2)	8.0(6)	6.2(6)	-4.9(2)

Table S4 Selected bond angles (°) and torsion angle (°) of the CN_7^- anions of compounds **7** - **10**

atoms	7a	7b	8	9	10a	10b	10c
N1–C1–N4	114.5(3)	114.0(2)	114.8(2)	114.0(4)	113.4(3)	114.0(3)	113.4(3)
N1–C1–N5	123.6(3)	123.8(3)	125.9(2)	126.3(4)	125.8(3)	126.6(3)	125.5(3)
N4–C1–N5	121.8(3)	122.3(3)	119.3(2)	119.7(4)	120.8(3)	119.4(3)	121.1(3)
C1–N5–N6	113.4(2)	114.0(2)	115.5(2)	113.7(4)	111.8(3)	114.8(3)	113.2(3)
N5–N6–N7	173.6(4)	171.9(3)	169.3(3)	170.7(5)	173.7(3)	169.7(4)	173.6(4)

N1–C1–N5–N6	-172.6(3)	9.3(4)	172.6(3)	5.4(7)	177.1(3)	175.4(3)	2.9(5)
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complete Ref. 56:

Gaussian 03, Revision C.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A.; Vreven, J. T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian Inc.: Pittsburgh PA, **2003**.